

# Many-body wavefunctions for normal liquid $^3\text{He}$

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We present new trial wave-functions which include 3-body correlations into the backflow coordinates and a 4-body symmetric potential. We show that our wavefunctions lower the energy enough to stabilize the ground state energies of normal liquid  $^3\text{He}$  in the unpolarized state at all pressures in agreement with experiment; however, quantitative discrepancies remain. Further, we include strong spin coupling into the Fermi liquid by adapting pairing wave functions. We demonstrate a new, numerically stable method to evaluate pairing functions which is also useful for Path Integrals calculations at low, but non-zero temperatures.

For the understanding and development of quantum many-body systems, liquid helium is a key test case due to its experimentally well-characterized low temperature phases and the simplicity of the helium interaction. The calculation of its thermodynamic and ground state properties is one of the most important benchmarks for microscopic theory and for the quantum Monte Carlo(QMC) simulation methods<sup>1,2,3,4</sup>. While QMC can calculate exact properties for bosonic systems, and has successfully been applied to calculate properties for liquid and solid  $^4\text{He}$ <sup>5,6</sup>, fermion systems are still challenging, since anti-symmetry leads to the so-called fermion sign problem. In general, no exact method is known which provides a solution for an extended fermion quantum system in two or three spatial dimensions.

To overcome the fermion-sign problem, most fermion QMC calculations rely on the fixed-node (FN) approximation where the nodes of a trial wavefunction,  $\psi_T$ , are imposed as a boundary condition on the many-body Schrödinger equation with the projector Diffusion Monte Carlo (DMC) method<sup>7</sup>. Since the nodal surfaces of the exact ground state wavefunction are, in general unknown, the energies of FN-DMC calculations are higher than the exact answer by a small but unknown amount. Progress in fermionic Monte Carlo calculations is, therefore, often connected to progress in constructing new types of trial wavefunctions. Actually, for homogeneous quantum systems, only a few types of different trial wavefunctions have been successfully applied within QMC, in particular for liquid  $^3\text{He}$ <sup>8,9,10,11</sup>.

Many calculations use the simplest possible nodal structure based on a Slater-Jastrow wavefunction

$$\psi_{SJ} = \det_{ki} \phi_k(\mathbf{r}_i) \exp[-U_J] \quad (1)$$

where  $\mathbf{r}_i$  are the positions of the  $N$  fermions ( $i = 1, \dots, N$ ). Antisymmetry is assured by a Slater determinant,  $\det_{ki} \phi_k(\mathbf{r}_i)$  of single particle orbitals  $\phi_k(\mathbf{r})$ , where  $k$  labels one of the  $N$  single particle orbitals and the Jastrow potential  $U_J[\mathbf{R}] = \sum_{ij} u(r_{ij})$ ,  $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$ , takes into account correlations ( $\mathbf{R}$  indicates its dependance on all the particle coordinates). Since it is symmetric with respect to particle exchange and real, it does not modify the nodes of the many-body wavefunction and, therefore, it does not influence the ground state energy within

a FN-DMC calculation.

Homogenous quantum systems play an important role in understanding many-body correlations, since for inhomogeneous systems, the Hartree-energy typically dominates the correlation energy. Translational invariance restricts the single particle orbitals to be plane waves with energies less than the Fermi level. This explains why the simple Fermi liquid Slater determinant gives accurate results, and, at the same time, it explains the difficulty in going beyond Slater-Jastrow without violating homogeneity.

Backflow<sup>12</sup> is one possibility to extend this type of wavefunction by including many-body correlations in the nodes<sup>13,14,15</sup> using a Slater determinant  $\det_{ki} \phi_k(\mathbf{q}_i^{BF})$  where the bare coordinates  $\mathbf{r}_i$  used in the Slater determinant of the Slater-Jastrow wavefunctions are replaced by dressed “quasi-particle” coordinates

$$\mathbf{q}_i^{BF} = \mathbf{r}_i + \mathbf{Y}_i \quad (2)$$

where  $\mathbf{Y}_k[\mathbf{R}] = \nabla_k \sum_{ij} y(r_{ij})$ . An additional symmetric 3-body potential,  $U_{3B}$ , is also added to the Jastrow part of the trial function

$$U_{3B} = \lambda_T \sum_i \mathbf{W}_i \mathbf{W}_i \quad (3)$$

with  $\mathbf{W}_k[\mathbf{R}] = \nabla_k \sum_{ij} w(r_{ij})$ <sup>16</sup>. The resulting backflow-3-body (BF-3) wavefunction,

$$\psi_{BF3} = \det_{ki} \phi_k(\mathbf{q}_i^{BF}) \exp \{-U_J - U_{3B}\}, \quad (4)$$

contains the unspecified functions  $u(r)$ ,  $w(r)$ , and  $y(r)$ ; these are determined either by analytical theories or by numerically minimizing the expectation value of the energy using simple analytical forms with free parameters. The backflow 3-body wavefunction (BF-3) has provided the most accurate results for the electron-gas<sup>17,18,19</sup> and for liquid  $^3\text{He}$ <sup>10,11,20,21</sup>. Spin-dependent correlations have been considered in Ref.<sup>22</sup>, but have found to be roughly equivalent to backflow.

However, the calculated liquid  $^3\text{He}$  energy and magnetic susceptibility is still in disagreement with experimental estimates<sup>20,21</sup>; the FN-DMC ground state energy

is higher by about 260mK. The prediction of the polarization energy is particularly unsatisfactory: within Variational Monte Carlo (VMC), the Slater-Jastrow wavefunction predicts a polarized fluid at zero pressure<sup>23</sup>, inclusion of three-body correlations results in a slight improvement, however, still largely unsatisfactory<sup>24</sup>. Backflow mainly affects the unpolarized state and therefore improves the estimate of the polarization energy. Only within FN-DMC is the unpolarized state stable at zero pressure, but the computed susceptibility is still too large, and at higher pressure, the unpolarized state becomes unstable<sup>21</sup>. Because liquid <sup>3</sup>He is such an important benchmark system, it is crucial to find what correlations are absent in the backflow-3-body wavefunctions.

Pairing wavefunctions, where the Slater determinant is replaced by the antisymmetrization of a pairing wavefunction  $\phi(r_i, r_j)$  has been suggested by Bouchaud and Lhuillier<sup>25</sup> to overcome this problem. In general, the antisymmetrization of a pairing functions leads to a pfaffian,  $\text{Pf}_{i,j}\phi(r_i, r_j)$  which reduces to a determinant for a  $M = 0$  (s-wave) pairing wavefunction. Recently, singlet pairing wavefunctions, have been applied to calculations on the BEC-BCS crossover of fermionic gases<sup>26,27,28</sup>. As far as the calculations on <sup>3</sup>He are concerned, spin-triplet pairing wavefunction with  $M = 1$  (p-wave) are promising, but it remains to be shown that they indeed provide lower energies than the backflow-3 body wavefunctions.

It is known experimentally that the ground state of <sup>3</sup>He is a *superfluid* with *spin triplet pairing*. The transition occurs around 1mK which is an estimate of the energy gap,  $\Delta$ . We expect that energy differences between the true superfluid ground state and the best Fermi liquid state are small, of order  $\Delta \sim 1\text{mK}$  and the introduction of a superfluid pairing wavefunction alone *can not resolve* the *energetic mismatch* between theory and experiment of order 260mK. Further, one expects that pairing only involves states close to the Fermi surface, e.g. states of momenta  $k$  with  $k_F - \delta k < k < k_F + \delta k$  where  $k = k_F$  at the Fermi surface and  $\delta k \sim 2m\Delta/k_F$  defines the typical coherence length  $\xi \sim \delta k^{-1}$  of the pairing wave function. In <sup>3</sup>He ( $k_F \sim 0.9\text{\AA}^{-1}$ ) one estimates  $\delta k \sim 10^{-2}\text{\AA}^{-1}$ , and the coherence length  $\xi \sim 100\text{\AA}$  exceeds by an order of magnitude the size of a typical simulation box,  $L$ , as  $L \sim 10\text{\AA}$  for a system of  $N = 66$  atoms. Strong correlations in helium in changing the bare mass into the effective mass hardly modify this conclusion. On the other hand size effects (for a non-degenerate ground state) will favor the normal state since the energy of a weakly bound state is increased when the size of the system is decreased. For these reasons, we mainly limit the discussion to the normal state.

In this paper, we propose new types of trial wavefunctions with explicit many-body character and use them to calculate the unpolarized ground state energy of <sup>3</sup>He at the maximum, intermediate, and the minimum densities of liquid <sup>3</sup>He. First, we introduce a three-particle backflow and 4-body correlations (3BF-4), as a natural extension of the backflow-3-body (BF-3) Fermi liquid

$\rho$ (nm <sup>-3</sup> )	wavefunction	$E_v(K)$	$\sigma^2$	$E_{DMC}(K)$
16.35	BF-3	-2.201(6)	23	-2.417(1)
	3BF-4	-2.284(3)	14	-2.438(1)
	S3BF-4	-2.294(3)	14	-2.432(4)
19.46	BF-3	-1.775(5)	26	-2.155(5)
	3BF-4	-1.905(4)	20	-2.174(3)
	S3BF-4	-1.945(4)	20	-2.182(4)
23.80	BF-3	-0.055(1)	65	-0.77 (2)
	3BF-4	-0.272(7)	53	-0.834(2)
	S3BF-4	-0.340(5)	49	-0.861(4)

TABLE I: Variational ( $E_v$ ) and FN-DMC energies ( $E_{DMC}$ ) in K/atom for a system of  $N = 66$  unpolarized <sup>3</sup>He atoms with periodic boundary conditions at two different densities;  $\sigma^2$  is the variance per atom; BF-3 are results of the backflow-3body wavefunction, 3BF-4 are the results presented here using an additional 3-body correlation for the backflow and an additional symmetric 4-body term, and S3BF-4 is the pairing form described below.

wavefunction. As in the case of backflow, the Slater-determinant is a function of quasi-particle coordinates, but a three-body correlation is added to the original backflow coordinate

$$\mathbf{q}_i^{3BF} = \mathbf{q}_i^{BF} + \hat{\mathbf{Q}}_i \mathbf{D}_i \quad (5)$$

where  $\hat{\mathbf{Q}}_i[R]$  is a tensor with generic elements  $\hat{\mathbf{Q}}_k[R]_{\alpha\beta} = \nabla_{k\alpha} \nabla_{k\beta} \sum_{ij} q(r_{ij}) + \delta_{\alpha\beta} \nabla_k^2 \sum_{ij} q'(r_{ij})$ , and  $\mathbf{D}_k[R] = \nabla_k \sum_{ij} d(r_{ij})$  is a vector. Furthermore, a symmetric 4-body potential is added to the Jastrow part of the trial function:

$$U_{4B} = \sum_i \mathbf{X}_i \hat{\mathbf{P}}_i \mathbf{X}_i \quad (6)$$

where  $\hat{\mathbf{P}}_i[R]$  is a tensor and  $\mathbf{X}_i$  a vector, analogous to  $\hat{\mathbf{Q}}$  and  $\mathbf{D}$ . The new trial wavefunction including 3-body backflow and a 4-body potential (3BF-4) is:

$$\psi_{3BF4} = \det_{kij} \phi_k(\mathbf{q}_i^{3BF}) \exp[-U_J - U_{3B} - U_{4B}]. \quad (7)$$

As in previous studies, we use gaussian functions as a basis for the 1-D functions arising in the wavefunction (such as  $q, q'$  and  $d$ ), and minimize a combination of energy and variance of the trial wavefunction within VMC. Results for a system of  $N = 66$  unpolarized <sup>3</sup>He atoms interacting with the recent Aziz-SAPT2 potential<sup>29,30</sup> with periodic boundary conditions are shown in table I<sup>31</sup>. To reduce finite size effects we have also performed twist averaging<sup>32</sup> and we have corrected size-effects in the potential energy. Results for different polarizations are given in table II. For comparison we have added the twist-averaged results of the backflow 3-body wavefunctions of Ref.<sup>21</sup> in table II and the corresponding results for periodic boundary conditions in table I.

The three densities 16.35, 19.46, and 23.80 atoms nm<sup>-3</sup> correspond to pressures equal to 0, 8.4, and 35.3 bar. The magnetic susceptibility,  $\chi/C$ , has been estimated in table III by assuming  $E = E_0 + \zeta^2/(2\chi/C) +$

$\rho$ (nm $^{-3}$ )	$\zeta$	$E_v(K)$ BF-3	$E_{DMC}(K)$ BF-3	$E_v(K)$ 3BF-4	$E_{DMC}(K)$ 3BF-4
16.35	0	-2.1633(9)	-2.3586(8)	-2.241(1)	-2.3802(4)
	0.242	-2.1614(9)	-2.3548(10)	-2.242(1)	-2.3743(1)
	0.485	-2.1753(9)	-2.3433(8)	-2.248(1)	-2.3633(6)
19.46	0	-1.7469(12)	-2.0685(13)	-1.863(1)	-2.0972(9)
	0.242	-1.7499(12)	-2.0623(13)	-1.873(1)	-2.0948(6)
	0.485	-1.7984(12)	-2.0807(11)	-1.905(1)	-2.1046(8)
23.80	0	-0.0184(20)	-0.6612(20)	-0.203(2)	-0.7094(9)
	0.242	-0.0229(21)	-0.6619(21)	-0.222(2)	-0.7093(11)

TABLE II: VMC and DMC energies of the BF-3 wavefunction of Ref. <sup>21</sup> and of the 3BF-4 wavefunction using twist averaged boundary conditions. Notations and units as in table I;  $\zeta$  is the polarization.

$\rho$ (nm $^{-3}$ )	$\chi/C(K^{-1})$ BF-3	$\chi/C(K^{-1})$ 3BF-4	$\rho_{exp}$ (nm $^{-3}$ )	$\chi_{exp}/C$ (K $^{-1}$ )
16.35	8(2)	4.5(5)	16.37	3.0
19.46	5(2)	8(3)	19.44	4.0
23.80	-	$ \chi/C  \gtrsim 14$	23.45	6.1

TABLE III: Magnetic susceptibility  $\chi/C$  in  $K^{-1}$ , where  $C$  is the molar Curie constant, estimated from the DMC calculations using the 3BF-4 wavefunction; experimental values<sup>33</sup> at densities  $\rho_{exp}$  are given for comparison.

$a_4\zeta^4$  where  $\zeta$  is the spin polarization. At the equilibrium density, inclusion of 3 and 4-body correlations reduce the magnetic susceptibility in agreement with the experimental value<sup>33</sup>. Away from equilibrium density,  $a_4$  becomes more important, and the estimate of  $\chi/C$  at the intermediate density is less reliable. Close to crystallization, the energy variation between the unpolarized and the partially polarized state for the 3BF-4 wavefunction is of the order of the uncertainty of the calculation. We have not performed calculations for the 100% polarized phase since backflow is already much less important than in the unpolarized phase<sup>22</sup>; similarly 3-body correlations mainly affect the unpolarized state<sup>24</sup>. Therefore, we do not expect significant corrections to the energies of the complete polarized state of the BF-3 trial function.

We have tried also different tensorial forms for a 4-body trial function, a 5-body trial function, as well as 4-body and k-dependent corrections to the quasi-particle coordinates without significant improvements (< 5mK). We cannot exclude the possibility that more effective optimization with more flexible functions would lead to significantly lower energy. This possibility, together with the application of the released node technique<sup>35</sup> is under current investigation.

We have also considered pairing wavefunctions. Simple functional forms (Gaussians) for the pairing functions (plus the Jastrow potential) have led to energies considerably higher than those from the BF-3 trial functions. Shell effects lead to large size effects and make a direct comparison of energies of triplet and singlet pairing wavefunctions problematic without a careful extrapolation to the thermodynamic limit. Since triplet pairing functions

did not show significant improvements over the singlet pairing, we restrict the pairing functions to spin-singlet pairing: the pfaffian reduces to a determinant and the antisymmetric part of the wavefunction is:

$$\det_{ij} \phi_s(\mathbf{r}_{i\uparrow} - \mathbf{r}_{j\downarrow}) \quad (8)$$

where  $\mathbf{r}_{i\uparrow}$  ( $\mathbf{r}_{i\downarrow}$ ) represents the coordinates of particle  $i$  with spin-up (down). Using a Gaussian form for  $\phi_s(r)$ , we have that the minimum energy orbital has a width as large as the simulation cell,  $L$ . In this case, the orbitals have to be periodized, which is most easily done using a Fourier sum. Optimization of the Fourier coefficients led to the limiting form of the Fermi liquid:

$$\phi_{FL}(r) = \sum_{k \leq k_F} e^{i\mathbf{k} \cdot \mathbf{r}} \quad (9)$$

We conclude that pairing of bounded singlet/triplet pairs does not improve the energy significantly, consistent with the small pairing energy in superfluid  $^3\text{He}$ .<sup>37</sup>

To go beyond the Fermi liquid trial function, we can use the singlet pairing wavefunction as a way of introducing strong spin-correlations:

$$\phi_s(r) = \sum_{k \leq k_F} e^{i\mathbf{k} \cdot \mathbf{r}[1+\eta(r)]} e^{-\nu(r)} \quad (10)$$

in the determinant of Eq. (8). Here  $\eta(r)$  and  $\nu(r)$  are localized functions vanishing at large particle separation. They introduce modulations and correlations in the pairing of opposite-spin atoms without affecting the long-range correlations of the Fermi-liquid determinant. They do not describe a bound state, so we do not expect them to describe a superfluid state, but they might be a precursor to superfluidity. However, the correlations between unlike spins turn out to be much stronger than introducing a spin-dependent backflow or Jastrow potential which have not been successful in lowering the energy. We also include backflow, 3-body backflow, 3-body, and 4-body potentials as discussed above:

$$\psi_{S3BF4} = \det_{i,j} \phi_s(\mathbf{q}_{i\uparrow}^{3BF} - \mathbf{q}_{j\downarrow}^{3BF}) e^{-U_J - U_{3B} - U_{4B}}. \quad (11)$$

As shown in table I, the energies are lowered by this wavefunction. By construction, this wavefunction does not affect the energy of the completely polarized state and, therefore, it stabilizes the unpolarized phase. We have not performed twist-averaging, but it is likely that the relative gain of the energy compared to the 3-body backflow wavefunction survives in the thermodynamic limit, but a more detailed study of the finite size extrapolation of this wavefunction remains to be done. In Ref.<sup>21</sup>, it was estimated that the 3-body potential together with the effect of higher order many body terms in the interparticle interactions raise the energy by  $\sim 140\text{mK}$ , and have to be added to the computed results when compared to the experimental energy<sup>36</sup>  $-2.481K$  at  $\rho = 16.35\text{nm}^{-3}$ . Even if the absolute energies are therefore still in disagreement

with experiments by  $\sim 240\text{mK}$  the agreement with the compressibility is considerably improved. Further, we expect a reduced magnetic susceptibility compared to the 3BF-4 wavefunctions, closer to the experimental values. At high density  $10 - 20\text{mK}$  might be still missing to stabilize completely the unpolarized phase. However, size effects are of the order of  $30\text{mK}$ , and a clear prediction would involve an extensive finite size study.

We briefly explain our method to evaluate the determinant of the pairing function in Eq.(11). A straightforward evaluation of the determinant of the matrix  $\Phi_{ij} = \phi_s(r_i, r_j)$  is numerically unstable in the limit where the wavefunction approaches a Fermi liquid, Eq. (9), because it becomes ill-conditioned; a direct evaluation of the determinant is dominated by round-off errors as the number of particles,  $N$ , increases. Let us consider the expansion of the pairing functions, into eigen-modes,  $\varphi_k(r)$ ,

$$\phi_s(r_i, r_j) = \sum_k d_k \varphi_k^*(r_i) \varphi_k(r_j) \quad (12)$$

where  $d_k$  is the occupation number of eigenstate  $k$ . For a Fermi liquid, the summation is dominated by  $N$  modes,  $k = 1, \dots, N$ . We introduce the matrices of the Slater-determinants of the Fermi Liquid,  $L_{ik} = \varphi_k^*(r_i)$ ,  $R_{ki} = \varphi_k(r_i)$ , and a diagonal matrix  $D_{kk'} = \delta_{k,k'} d_k$ , and write Eq.(12) as a matrix,

$$\Phi = LDR + M = LD^{1/2} \left( 1 + \tilde{M} \right) D^{1/2} R \quad (13)$$

with  $M_{ij} = \sum_{k>N} d_k \varphi_k^*(r_i) \varphi_k(r_j)$ , and  $\tilde{M} =$

$L^{-1} D^{-1/2} M D^{-1/2} R^{-1}$ . Now, the determinant of Eq.(13) can be written as:

$$\det \Phi = \det L \det D \det R \det(1 + \tilde{M}) \quad (14)$$

and involves only the usual Slater determinants,  $\det L$ ,  $\det R$  and their inverses which are well-behaved. The matrix  $\tilde{M}$  is typically much more rapidly decaying in space and a numerical evaluation of the terms on the rhs of Eq. (14) is numerically stable, including all limiting cases. This method is not restricted to spin singlet/triplet pairing, but it is also useful to calculate finite temperature density matrices well below the Fermi-temperature where the same problem of extremely ill conditioned determinants occurs.

In conclusion, we have found 3-body and 4-body correlations improving the energy and the magnetic susceptibility of liquid  $^3\text{He}$ . We expect that the new terms will be important to calculate the Fermi liquid parameters in strongly correlated liquids such as liquid  $^3\text{He}$  and the electron gas, the polarization transition of the electron gas close to Wigner crystallization and related systems. The method to calculate pairing function close to the Fermi liquid should further allow the study the very dilute limit of a BCS gas.

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<sup>1</sup> W.L. McMillan, Phys. Rev. **138**, A442 (1965).  
<sup>2</sup> D. Levesque, T. Khiet, D. Schiff, and L. Verlet, Orsay report (unpublished) (1965).  
<sup>3</sup> M.H. Kalos, D. Levesque, and L. Verlet, Phys. Rev. **A9**, 2178 (1974).  
<sup>4</sup> D. Ceperley, G.V. Chester, and M.H. Kalos, Phys. Rev. **B16**, 3081 (1977).  
<sup>5</sup> P.A. Whitlock, D.M. Ceperley, G.V. Chester, and M.H. Kalos, Phys. Rev. **B19**, 5598 (1979).  
<sup>6</sup> D. M. Ceperley, Rev. Mod. Phys. **67**, 279 (1995).  
<sup>7</sup> P.J. Reynolds, D.M. Ceperley, B.J. Alder, and W.A. Lester, J. Chem. Phys. **77**, 5593 (1982).  
<sup>8</sup> M. A. Lee, K. E. Schmidt, M.H. Kalos, and G. V. Chester, Phys. Rev. Lett. **46**, 728 (1981).  
<sup>9</sup> K. E. Schmidt, M. A. Lee, M. H. Kalos, and G.V. Chester, Phys. Rev. Lett. **47**, 807 (1981).  
<sup>10</sup> R. M. Panoff and J. Carlson, Phys. Rev. Lett. **62**, 1130 (1989).  
<sup>11</sup> J. Casulleras and J. Boronat, Phys. Rev. Lett. **84**, 3121 (2000).  
<sup>12</sup> R. P. Feynman and M. Cohen, Phys. Rev. **102**, 1189 (1956).  
<sup>13</sup> V. R. Pandharipande and N. Itoh, Phys. Rev. A **8**, 2564 (1973).  
<sup>14</sup> K. E. Schmidt and V. R. Pandharipande, Phys. Rev. B **19**, 2504 (1979).  
<sup>15</sup> E. Manousakis, S. Fantoni, V. R. Pandharipande, and Q. N. Usmani, Phys. Rev. B **28**, 3770 (1983).  
<sup>16</sup> The 3-body potential of Eq. (3) includes “self-terms” of the form  $\sum_{ij} [\nabla_i w(r_{ij})]^2$  which should be subtracted out. To simplify the notation self terms are assumed to be subtracted in the following.  
<sup>17</sup> Y. Kwon, D. M. Ceperley and R. M. Martin, Phys. Rev. B **48**, 12037 (1993).  
<sup>18</sup> Y. Kwon, D. M. Ceperley and R. M. Martin, Phys. Rev. B **58**, 6800 (1998).  
<sup>19</sup> M. Holzmann, D. M. Ceperley, C. Pierléoni and K. Esler, Phys. Rev. E **68**, 046707 (2003).  
<sup>20</sup> S. Moroni, S. Fantoni, and G. Senatore, Phys. Rev. B **52**, 13547 (1995).  
<sup>21</sup> F.H. Zong, D.M. Ceperley, S. Moroni, and S. Fantoni, Mol. Phys. **101**, 1705 (2003).  
<sup>22</sup> S. A. Vitiello, K. E. Schmidt, and S. Fantoni, Phys. Rev. B **55**, 5647 (1997).  
<sup>23</sup> D. Levesque, Phys. Rev. **21**, 5159 (1981).  
<sup>24</sup> C. Lhuillier and D. Levesque, Phys. Rev. B **23**, 2203 (1981).  
<sup>25</sup> J.P. Bouchaud and C. Lhuillier, *Spin Polarized Quantum Systems*, edited by S. Stringari, Singapore: World Scientific (1988).  
<sup>26</sup> J. Carlson, S. Y. Chang, V. R. Pandharipande, and K. E.

Schmidt, Phys. Rev. Lett. **91**, 050401 (2003).

<sup>27</sup> S. Y. Chang, V. R. Pandharipande, J. Carlson, and K. E. Schmidt, Phys. Rev. **A70**, 043602 (2004).

<sup>28</sup> G. E. Astrakharchik, J. Boronat, J. Casulleras, and S. Giorgini, Phys. Rev. Lett. **93**, 200404 (2004).

<sup>29</sup> T. Korona, H.L. Williams, R. Bukowski, B. Jeziorski, and K. Szakewicz, J. Chem. Phys. **106**, 5109 (1997).

<sup>30</sup> A.R. Janzen and R.A. Aziz, J. Chem. Phys. **107**, 914 (1997).

<sup>31</sup> Size-effects in the potential energy raise the energy by  $\sim 10\text{mK}$  at low density and  $\sim 30\text{mK}$  at high density<sup>21</sup>; 3body potential corrections remain roughly unaffected.

<sup>32</sup> C. Lin, F. H. Zong, and D. M. Ceperley, Phys. Rev. **E64**, 016702 (2001).

<sup>33</sup> V. Goudon et al. (CRTBT Grenoble) to be published; the experimental magnetic susceptibilities are roughly 5% higher than those of Ref.<sup>34</sup>.

<sup>34</sup> H. Ramm, P. Pedroni, J.R. Thompson, and H. Meyer, J. of Low Temp. Phys. **2**, 539 (1970).

<sup>35</sup> D. M. Ceperley and B. J. Alder, J. Chem. Phys. **81**, 5833 (1984).

<sup>36</sup> R.A. Aziz and R.K. Pathria, Phys. Rev. **A7** 809 (1973); the energy at zero pressure is from L. Reesink, PhD thesis, University of Leiden (2001).

<sup>37</sup> Finite size effects are important as one has to express the pairing function in Fourier space for weakly bound pairs and the discrete level spacing of the finite system dominates.